

Thermoelectric efficiency of critical quantum junctions

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(Dated: October 31, 2013)

We derive the efficiency at maximal power of a scale-invariant (critical) quantum junction in exact form. Both Fermi and Bose statistics are considered. We show that time-reversal invariance is spontaneously broken. For fermions we implement a new mechanism for efficiency enhancement above the Curzon-Ahlborn bound, based on a shift of the particle energy in each heat reservoir, proportional to its temperature. In this setting fermionic junctions can even reach at maximal power the Carnot efficiency. Bosonic junctions at maximal power turn out to be less efficient than fermionic ones.

PACS numbers: 05.70.Ln, 73.63.Nm, 72.15.Jf

There is recently much interest in the study of thermoelectric phenomena in nanoscale devices and in particular, in nanoscale engines. The efficiency of such engines is a fascinating physical problem. As is well known, one relevant parameter for studying this problem is the efficiency $\eta(P_{\max})$ at maximal power P_{\max} . In the context of classical linear endoreversible thermodynamics (irreversible heat transfer) it has been shown [1, 2] that

$$\eta(P_{\max}) \leq 1 - \sqrt{\frac{T_2}{T_1}} \equiv \eta_{CA}, \quad (1)$$

where $T_1 > T_2$ are the temperatures of the two reservoirs, needed for running the engine. The inequality (1) is known as Curzon-Ahlborn (CA) bound. In a series of recent papers [3]-[8] it has been proposed that at the quantum level $\eta(P_{\max})$ might be enhanced in principle above η_{CA} by means of an *explicit* breaking of time-reversal symmetry. For this purpose, the authors of [3]-[7] considered in the linear response regime a three-terminal setup with one probe terminal and a magnetic field, which breaks down time-reversal. A generalization of this idea to multi-terminal systems has also been studied [8].

In the present paper we investigate the efficiency of quantum Schrödinger junctions with both Fermi and Bose statistics. We demonstrate that when the interaction, driving the system away from equilibrium is *scale invariant* (critical), one can go beyond the linear response approximation and derive $\eta(P_{\max})$ in exact form. Time reversal invariance is *spontaneously* broken, which provides in the quantum world an attractive alternative to the explicit breaking in [3]-[7]. For fermions we propose and investigate a new mechanism for efficiency enhancement above η_{CA} , based on a shift of the energy in the heat reservoirs proportional to their temperature. With an appropriate shift, fermionic junctions can reach at maximal power even the Carnot efficiency η_C . Analogous behavior has been observed [9] in the stochastic model of an isothermal engine. At maximal power the bosonic junctions are less efficient and do not attain $\eta_C/2$.

The system: The scheme of the junction, considered in this Letter, is shown in Fig. 1. The two thermal reser-

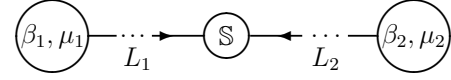


FIG. 1: (Color online) Schematic picture of the junction with two heat reservoirs connected via two leads L_1 and L_2 to the scattering matrix \mathbb{S} .

voirs at (inverse) temperature β_i and chemical potential μ_i are connected with two semi-infinite leads through a point-like interaction characterized by a unitary scattering matrix \mathbb{S} . The leads L_i are modeled by two half-lines with local coordinates $\{(x, i) : x < 0, i = 1, 2\}$, \mathbb{S} being localized at $x = 0$. The system is away from equilibrium provided that \mathbb{S} has a non-vanishing transmission amplitudes and β_1 and/or μ_1 differ from β_2 and/or μ_2 . The dynamics is fixed by the Schrödinger equation

$$\left(i\partial_t + \frac{1}{2m}\partial_x^2 - \frac{a}{\beta_i} \right) \psi(t, x, i) = 0, \quad (2)$$

where m is the mass and a is a dimensionless real parameter. We show in what follows that the term a/β_i (a temperature dependent potential), generating a shift in the dispersion relations

$$\omega_i(k) = \frac{k^2}{2m} + \frac{a}{\beta_i} \quad (3)$$

of the particles in the two heat baths, affects $\eta(P_{\max})$.

We adopt a field theory formulation. Accordingly, the Schrödinger field $\psi(t, x, i)$ with (Fermi) Bose statistics satisfies the standard equal-time canonical (anti)commutation relations. The interaction at the point $x = 0$ is fully codified in the boundary condition

$$\lim_{x \rightarrow 0^-} \sum_{j=1}^2 [\varrho(\mathbb{I} - \mathbb{U})_{ij} + i(\mathbb{I} + \mathbb{U})_{ij} \partial_x] \psi(t, x, j) = 0, \quad (4)$$

where \mathbb{U} is an arbitrary 2×2 unitary matrix and $\varrho \in \mathbb{R}$ is a parameter with dimension of mass. This is [11, 12] the most general boundary condition, implying the self-adjointness of the operator $-\partial_x^2$ and thus of the Hamiltonian of the system. The scattering matrix, associated with the point-like interaction generated by (4), is [11, 12]

$$\mathbb{S}(k) = -\frac{[\varrho(\mathbb{I} - \mathbb{U}) - k(\mathbb{I} + \mathbb{U})]}{[\varrho(\mathbb{I} - \mathbb{U}) + k(\mathbb{I} + \mathbb{U})]}, \quad (5)$$

which is unitary and satisfies $\mathbb{S}^*(k) = \mathbb{S}(-k)$ (Hermitian analyticity) [10] and $\mathbb{S}(\varrho) = \mathbb{U}$. Summarizing, the scattering matrix (5) describes all possible point-like interactions, which generate a unitary time evolution of ψ . Junctions with more than two terminals can be treated [13] along the same lines.

The non-equilibrium steady state $\Omega_{\beta,\mu}$: Following the pioneering work of Landauer [14] and Büttiker [15], non-equilibrium systems of the type shown in Fig. 1 have been extensively investigated (see [16] and references therein). We use here an algebraic construction [17] of the Landauer-Büttiker (LB) steady state $\Omega_{\beta,\mu}$ for the problem (2-5), allowing to establish explicitly the spontaneous breakdown of time-reversal symmetry. Referring for the details to [17], we report only the two-point *non-equilibrium* correlation function, needed in what follows. Denoting by $\langle \cdots \rangle_{\beta,\mu}$ the expectation value in the state $\Omega_{\beta,\mu}$, one has

$$\begin{aligned} \langle \psi^*(t_1, x_1, i) \psi(t_2, x_2, j) \rangle_{\beta,\mu} &= \int_0^\infty \frac{dk}{2\pi} e^{i\omega_i(k)t_1 - i\omega_j(k)t_2} \\ &\left[e^{ikx_{12}} \delta_{ji} d_i^\pm(k) + e^{-ikx_{12}} \sum_{l=1}^2 \mathbb{S}_{jl}(k) d_l^\pm(k) \mathbb{S}_{li}^*(k) \right. \\ &\left. e^{ik\tilde{x}_{12}} \mathbb{S}_{ji}(k) d_i^\pm(k) + e^{-ik\tilde{x}_{12}} d_j^\pm(k) \mathbb{S}_{ji}^*(k) \right], \end{aligned} \quad (6)$$

where $x_{12} = x_1 - x_2$, $\tilde{x}_{12} = x_1 + x_2$ and

$$d_i^\pm(k) = \frac{1}{e^{\beta_i[\omega_i(k) - \mu_i]} \pm 1} \quad (7)$$

is the Fermi/Bose distribution in the i -th reservoir. The correlation function (6) is essentially the only input for deriving the efficiency $\eta(P_{\max})$ below.

Time-reversal: It is natural to consider the time-reversal symmetry as a quantum counterpart of classical reversibility, thus interpreting its breakdown as *quantum irreversibility*. The equation of motion (2) is invariant under the conventional time-reversal operation

$$T\psi(t, x, i)T^{-1} = -\chi_T\psi(-t, x, i), \quad |\chi_T| = 1, \quad (8)$$

T being an *anti-unitary* operator. The same is true for the boundary condition (4), provided that \mathbb{U} (and therefore $\mathbb{S}(k)$) is symmetric [18]. In spite of the fact that in this case both dynamics and boundary condition preserve the time-reversal symmetry, it turns out [17] that the LB

state $\Omega_{\beta,\mu}$ breaks it down. The simplest way to detect this spontaneous breakdown is to use (6) and observe that

$$\begin{aligned} \langle \psi^*(t_1, x_1, i) \psi(t_2, x_2, j) \rangle_{\beta,\mu} &\neq \\ \langle \psi^*(-t_2, x_2, j) \psi(-t_1, x_1, i) \rangle_{\beta,\mu}, \end{aligned} \quad (9)$$

implying $T\Omega_{\beta,\mu} \neq \Omega_{\beta,\mu}$. The above argument shows that time-reversal is broken in the LB state $\Omega_{\beta,\mu}$ independently on the presence or absence of magnetic field or other explicitly breaking terms. This fact should not be surprising because $\Omega_{\beta,\mu}$ is a non-equilibrium state.

Thermoelectric transport in $\Omega_{\beta,\mu}$: The particle and energy currents are given by

$$j_x(t, x, i) = \frac{i}{2m} [\psi^*(\partial_x \psi) - (\partial_x \psi^*)\psi](t, x, i), \quad (10)$$

$$\begin{aligned} \theta_{xt}(t, x, i) &= \frac{1}{4m} [(\partial_t \psi^*)(\partial_x \psi) + (\partial_x \psi^*)(\partial_t \psi) \\ &- (\partial_t \partial_x \psi^*)\psi - \psi^*(\partial_t \partial_x \psi)](t, x, i). \end{aligned} \quad (11)$$

Inserting (10,11) in the correlator (6), one gets in the limit $x_1 \rightarrow x_2 = x$ the Landauer-Büttiker expressions

$$\begin{aligned} J_i^N &\equiv \langle j_x(t, x, i) \rangle_{\beta,\mu} = \\ &\int_0^\infty \frac{dk}{2\pi} \frac{k}{m} \sum_{j=1}^2 [\delta_{ij} - |\mathbb{S}_{ij}(k)|^2] d_j^\pm(k), \end{aligned} \quad (12)$$

$$\begin{aligned} J_i^E &\equiv \langle \theta_{xt}(t, x, i) \rangle_{\beta,\mu} = \\ &\int_0^\infty \frac{dk}{2\pi} \frac{k}{m} \sum_{j=1}^n [\delta_{ij} - |\mathbb{S}_{ij}(k)|^2] \omega_j(k) d_j^\pm(k). \end{aligned} \quad (13)$$

We stress that the expectation values (12,13) in the state $\Omega_{\beta,\mu}$ are exact and satisfy Kirchhoff's rule. No approximations (like linear response theory) have been used.

Scale invariance: The k -integration in (12,13) with general \mathbb{S} -matrix of the form (5) cannot be performed in closed analytic form. For this reason it is instructive to select among (5) the *scale-invariant* matrices, which incorporate the universal features of the system while being simple enough to be analyzed explicitly. These so called *critical points* of the set (5), are fully classified [19]. One has two isolated points $\mathbb{S} = \pm \mathbb{I}$ and the family

$$\mathbb{S}^U = U \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} U^*, \quad U \in U(2), \quad (14)$$

which is the orbit of the matrix $\text{diag}(1, -1)$ under the adjoint action of the unitary group $U(2)$. The transport for $\mathbb{S} = \pm \mathbb{I}$ is trivial because in this case the leads L_i are actually disconnected. So, we are left with (14) for which the k -integration in (12,13) is easily performed. From now on we consider the Fermi and Bose statistics separately.

Exact efficiency-fermions: With the Fermi distribution and the S-matrix (14) one infers from (12,13)

$$J_1^N = \frac{|\mathbb{S}_{12}^U|^2}{2\pi} \left[\frac{1}{\beta_1} \ln(1 + e^{\beta_1 \mu_1 - a}) - \frac{1}{\beta_2} \ln(1 + e^{\beta_2 \mu_2 - a}) \right] \quad (15)$$

$$J_1^E = \frac{|\mathbb{S}_{12}^U|^2}{2\pi} \left[\frac{a}{\beta_1^2} \ln(1 + e^{\beta_1 \mu_1 - a}) - \frac{a}{\beta_2^2} \ln(1 + e^{\beta_2 \mu_2 - a}) - \frac{1}{\beta_1^2} \text{Li}_2(-e^{\beta_1 \mu_1 - a}) + \frac{1}{\beta_2^2} \text{Li}_2(-e^{\beta_2 \mu_2 - a}) \right], \quad (16)$$

Li_2 being the dilogarithm function. By Kirchhoff's rule, $J_2^N = -J_1^N$ and $J_2^E = -J_1^E$. We stress that at criticality the whole information about the interaction, driving the system away from equilibrium, factorizes in the transmission probability $|\mathbb{S}_{12}^U|^2$ in front of the expectation values of the currents. This remarkable simplification allows us to compute the efficiency

$$\eta = \frac{(\mu_2 - \mu_1)J_1^N}{J_1^Q}, \quad J_1^Q = J_1^E - \mu_1 J_1^N, \quad (17)$$

exactly, J_i^Q being the heat currents. For this purpose we assume $\beta_2 > \beta_1$ and introduce the variables

$$\lambda_i = -\beta_i \mu_i \quad r = \beta_1 / \beta_2 \in [0, 1]. \quad (18)$$

Then, using (15), the electric power takes the form

$$P(\lambda_1, \lambda_2, r; a) = (\mu_2 - \mu_1)J_1^N = \frac{|\mathbb{S}_{12}^U|^2}{2\pi\beta_1^2} (\lambda_1 - r\lambda_2) \times [\ln(1 + e^{-\lambda_1 - a}) - r \ln(1 + e^{-\lambda_2 - a})]. \quad (19)$$

Let us derive now $\eta(P_{\max})$. We maximize (19) by varying λ_1 and λ_2 for fixed but arbitrary r and a . From $\partial_{\lambda_1} P = \partial_{\lambda_2} P = 0$ one can deduce that the extrema of (19) are localized at $\lambda_1 = \lambda_2 \equiv \lambda$, which satisfies the r -independent equation

$$\lambda - (1 + e^{\lambda + a}) \ln(1 + e^{-\lambda - a}) = 0. \quad (20)$$

One can also show that for $a \in \mathbb{R}$ the equation (20) has a unique solution λ_a , leading to maximal P . Inserting this information in (11,17,19), one gets

$$\eta_f(P_{\max}) = \frac{(1-r)\lambda_a \ln(1 + e^{-\lambda_a - a})}{(\lambda_a + a + ar) \ln(1 + e^{-\lambda_a - a}) - (1+r)\text{Li}_2(-e^{-\lambda_a - a})}, \quad (21)$$

which represents our main result. Notice that $\eta_f(P_{\max})$ vanishes in the isothermal limit $r \rightarrow 1$.

In order to clarify the role of the parameter $a \in \mathbb{R}$, we investigate the entropy production

$$\dot{S} \equiv (\beta_2 - \beta_1)J_1^Q - (\mu_2 - \mu_1)\beta_2 J_1^N. \quad (22)$$

At maximal power one finds for fermions

$$\dot{S}(a) = \frac{|\mathbb{S}_{12}^U|^2(1+r)(1-r)^2}{2\pi r \beta_1} \times [a \ln(1 + e^{-\lambda_a - a}) - \text{Li}_2(-e^{-\lambda_a - a})], \quad (23)$$

implying the existence of a point $a_f = -1.1628\dots$, such that $\dot{S}(a) \geq 0$ for $a \geq a_f$ and $\dot{S}(a_f) = 0$. On the other hand, using (16) and (23), one obtains the following relation between entropy production and energy flow at maximal power

$$J_1^E(a) = \frac{r}{\beta_1(1-r)} \dot{S}(a). \quad (24)$$

Combining these results with the orientation of the leads L_i in Fig. 1, we conclude that the energy flow is in the direction $1 \rightarrow 2$ for $a > a_f$ and $2 \rightarrow 1$ for $a < a_f$. Therefore, since $T_1 > T_2$, our junction operates as a thermoelectric engine for $a > a_f$. It turns out that for $a < a'_f = -3.5890\dots < a_f$ not only the energy flow J_1^E , but also the heat flow J_1^Q is in the direction $2 \rightarrow 1$ (for any $r \in [0, 1]$) and thus our device works as refrigerator.

Let us study in detail the behavior of the junction as a thermoelectric engine. For this purpose one solves numerically the equation (20) for fixed $a \geq a_f$ and plugs the pair (a, λ_a) in (21). The picture, emerging from this analysis, is displayed in Fig. 2. There exists a critical value

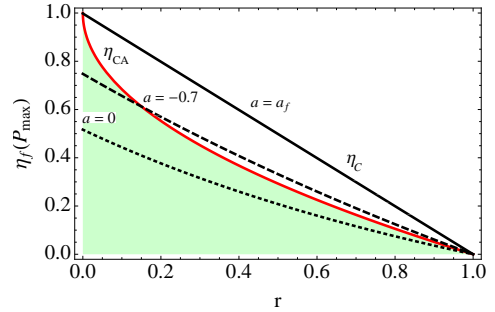


FIG. 2: (Color online) The CA bound (continuous red line) compared to $\eta_f(P_{\max})$ for $a = 0$ (dotted line), $a = -0.7$ (dashed line) and $a = a_f$ (continuous black line).

$a_c = -0.4978\dots$, such that $\eta_f(P_{\max}) < \eta_{CA}$ for all $a > a_c$. The conventional Schrödinger junction $a = 0$ is in this range. For $a_f \leq a < a_c$ one has $\eta_f(P_{\max}) > \eta_{CA}$ in some interval of r , as shown in Fig. 2 for $a = -0.7$. Because of (21) and (23), $\dot{S}(a_f) = 0$ implies that $\eta_f(P_{\max})$ equals precisely the Carnot efficiency $\eta_C = 1 - r$ at $a = a_f$.

From Fig. 2 one can deduce also that the enhancement can be detected in linear response theory (i.e. in the neighborhood of $r = 1$) as well. In fact, for $a \neq 0$ the associated Onsager matrix is not symmetric, which is a necessary condition for enhancement above η_{CA} .

Exact efficiency-bosons: For bosons the computation is totally analogous, except for the presence of a singularity in the integrand of (12,13) at $k^2 = -2m(\lambda_i + a)/\beta_i$. In

order to exclude it from the range of integration, we have to assume $\lambda_i + a > 0$. The bosonic counterparts of (20,21) are

$$\lambda - (1 - e^{\lambda+a}) \ln(1 - e^{-\lambda-a}) = 0, \quad \lambda + a > 0, \quad (25)$$

$$\eta_b(P_{\max}) = \frac{(1-r)\lambda_a \ln(1 - e^{-\lambda_a-a})}{(\lambda_a + a + ar) \ln(1 - e^{-\lambda_a-a}) - (1+r)\text{Li}_2(e^{-\lambda_a-a})}, \quad (26)$$

where λ_a satisfies (25). The study of equation (25) shows that for $a < a_b = -0.1792\dots$ there is no (real) solution for λ . There is one solution of (25) for $a = a_b$, which is a saddle point of the power P . In the interval $a_b < a \leq 0$ there are two solutions, one of which being a maximum of P . Finally, for $a > 0$ there is one solution, which also leads to maximal P . Summarizing, for each $a > a_b$ there exist λ_a satisfying both conditions (25) and giving a maximal power. Moreover, the entropy production (22) for bosons is positive in this range.

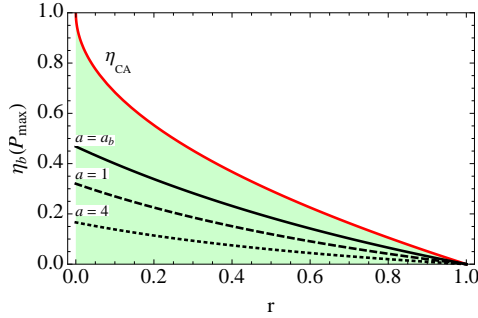


FIG. 3: (Color online) The CA bound (continuous red line) compared to $\eta_b(P_{\max})$ for $a = 4$ (dotted line), $a = 1$ (dashed line) and $a = a_b$ (continuous black line).

For illustration we have plotted in Fig. 3 the efficiency $\eta_b(P_{\max})$ for some values of the control parameter a . It turns out that $\eta_b(P_{\max})$ never exceeds η_{CA} in the allowed domain $a > a_b$. At maximal power the bosonic junctions behave therefore differently from the fermionic ones. We stress that the condition (25) is essential for this conclusion. If we release this condition, there exist points in the (a, λ) -plane (e.g. $(a = -1, \lambda = 28)$) with positive entropy production, in which also the bosonic efficiency becomes larger than η_{CA} and approaches η_C . However the power, delivered in these points, is not maximal.

Comparison with other bounds: For classical engines, which can reach the Carnot efficiency η_C in the reversible limit, the following upper and lower bounds

$$\frac{1}{2}\eta_C \equiv \eta_- \leq \eta(P_{\max}) \leq \eta_+ \equiv \frac{\eta_C}{2 - \eta_C}, \quad (27)$$

have been established in [20]-[22] without referring to linear response theory. For comparison with the CA bound

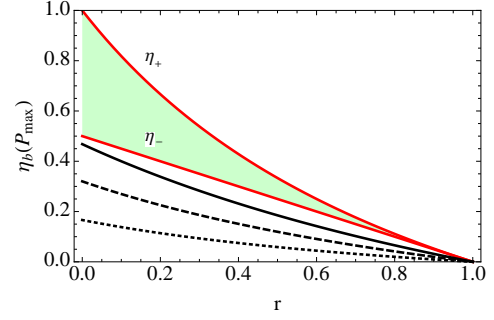


FIG. 4: (Color online) The η_{\pm} bounds (continuous red lines) compared to $\eta_b(P_{\max})$ for the same values of a as in Fig.3.

we observe that $\eta_- \leq \eta_{CA} \leq \eta_+$. Since $\eta_f(P_{\max}) = \eta_C$ for $a = a_f$, the fermion efficiency exceeds for appropriate values of a not only η_{CA} , but also η_+ . For bosonic junctions one has instead $\eta_b(P_{\max}) < \eta_-$ for all allowed values $a \geq a_b$, as illustrated in Fig. 4.

Conclusions: We derived and analyzed systematically the exact efficiency $\eta(P_{\max})$ for critical Schrödinger junctions in the Landauer-Büttiker steady state. Provided that the transmission probability between the two reservoirs does not vanish, the intensity of the interaction in the junction is irrelevant for $\eta(P_{\max})$ in the critical regime. Quantum irreversibility is implemented in our framework by a spontaneous breaking of time-reversal symmetry. We discovered that such a breaking is compatible with vanishing entropy production for certain value of the parameter a . In fact, in the fermion case $\dot{S}(a_f) = 0$, implying that $\eta_f(P_{\max})$ reaches the Carnot efficiency. The same mechanism works for bosons as well, but the corresponding value of a in this case is not in the regime of maximal power. Further clarifying the role of the parameter a and its impact on other physical observables (maximal efficiency, quantum noise,...) represents an interesting subject for future investigations.

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